

Listing of Model Species

Name	Description
Constant Species.	
O2	Oxygen
M	Air
H2O	Water
HV	Light
Active Inorganic Species.	
O3	Ozone
NO	Nitric Oxide
NO2	Nitrogen Dioxide
NO3	Nitrate Radical
N2O5	Nitrogen Pentoxide
HONO	Nitrous Acid
HNO3	Nitric Acid
HNO4	Peroxynitric Acid
HO2H	Hydrogen Peroxide
Active Radical Species and Operators.	
HO.	Hydroxyl Radicals
HO2.	Hydroperoxide Radicals
C-O2.	Methyl Peroxy Radicals
RO2.	Operator to Calculate Total Higher Organic Peroxy Radicals.
CCO-O2.	Acetyl Peroxy Radicals
RCO3.	Operator to Calculate Total Higher Acetyl Peroxy Radicals
Steady State Peroxy Radical Species or Operators	
RO2-R.	Peroxy Radical Operator representing NO to NO2 conversion with HO2 formation.
RO2-N.	Peroxy Radical Operator representing NO consumption with organic nitrate formation.
RO2-XN.	Peroxy Radical Operator representing NO consumption with formation of organic nitrates which are represented as unreactive.
RO2-NP.	Peroxy Radical Operator representing NO consumption with nitrophenol formation
R2O2.	Peroxy Radical Operator representing NO to NO2 conversion.
RCO-O2.	Peroxy Propionyl and higher peroxy acyl Radicals
HCOCO-O2.	Peroxyacyl radical formed from Glyoxal
BZCO-O2.	Peroxyacyl radical formed from Aromatic Aldehydes
MA-RCO3.	Peroxyacyl radicals formed from methacrolein and other acroleins.
[radical]	One such operator for each of the above steady state peroxy radical species or operators: Operator used to represent the reactions of the radical after its contribution to RO2. or RCO3. formation has already been taken into account.
Other Steady State Radical Species	
O3P	Ground State Oxygen Atoms
O*1D2	Excited Oxygen Atoms
C-O.	Methoxy Radicals
TBU-O.	t-Butoxy Radicals

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Name	Description
BZ-O.	Phenoxy Radicals
BZ(NO ₂)-O.	Nitro-substituted Phenoxy Radical
HOCOO.	Radical formed when Formaldehyde reacts with HO ₂

PAN and PAN Analogues

PAN	Peroxy Acetyl Nitrate
PAN2	PPN and other higher alkyl PAN analogues
GPAN	PAN analogue formed from Glyoxal
PBZN	PAN analogues formed from Aromatic Aldehydes
MA-PAN	PAN analogue formed from Methacrolein

Explicit Reactive Organic Product Species

CO	Carbon Monoxide
HCHO	Formaldehyde
MEOH	Methanol
COOH	Methyl Hydroperoxide
CCHO	Acetaldehyde
ACET	Acetone
GLY	Glyoxal
MGLY	Methyl Glyoxal
BACL	Biacetyl
ACROLEIN	Acrolein
METHACRO	Methacrolein
MVK	Methyl Vinyl Ketone
PHEN	Phenol

Lumped Reactive Organic Product Species

ROOH	Lumped higher organic hydroperoxides
RCHO	Lumped C ₃ + Aldehydes
MEK	Ketones and other non-aldehyde oxygenated products which react with OH radicals slower than 5×10^{-12} cm ³ molec ⁻² sec ⁻¹
PROD2	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than 5×10^{-12} cm ³ molec ⁻² sec ⁻¹
RNO ₃	Organic Nitrates
CRES	Cresols
BALD	Aromatic aldehydes (e.g., benzaldehyde)
NPHE	Nitrophenols
DCB1	Reactive Aromatic Fragmentation Products represented by 2-butene 1,3-dial.
DCB2	Reactive Aromatic Fragmentation Products which photolyze with alpha-dicarbonyl-like action spectrum.
DCB3	Reactive Aromatic Fragmentation Products which photolyze with acrolein action spectrum.
DCB4	Reactive Aromatic Fragmentation Products which do not photolyze rapidly.
ISOPROD	Lumped isoprene product species

Non-Reacting Species

CO ₂	Carbon Dioxide
XC	Lost Carbon
XN	Lost Nitrogen

Listing of Model Species

Name	Description
H2	Hydrogen
Low Reactivity Compounds or Unknown Products Represented as Unreactive	
HCOOH	Formic Acid
CCO-OH	Acetic Acid
RCO-OH	Higher organic acids
CCO-OOH	Peroxy Acetic Acid
RCO-OOH	Higher organic peroxy acids
CONO2	Methyl Nitrate
HCHO2-STAB	Stabilization products from the HCHO2 Crigiee biradical
CCHO2-STAB	Stabilization products from the CH3CHO2 Crigiee biradical
RCHO2-STAB	Stabilization products from Other Crigiee biradicals
NROG	Unspecified Unreactive Carbon
Primary Organics Represented explicitly	
CH4	Methane
ISOPRENE	Isoprene

SAPRC-99 Base Mechanism as of 1/9/99

Label	Rate Parameters [a]				Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea	B		
Inorganic Reactions						
1		Phot Set= NO2			1,2	NO2 + HV = NO + O3P
2	5.91e-34	5.91e-34	0.00	-2.8	3	O3P + O2 + M = O3 + M
3	8.34e-15	8.00e-12	4.09		4,5	O3P + O3 = #2 O2
4	1.00e-31	1.00e-31	0.00	-1.6	6,7,5	O3P + NO + M = NO2 + M
5	9.70e-12	6.50e-12	-0.24		4,5	O3P + NO2 = NO + O2
6	1.79e-12	Falloff, F=0.80			4,7,5	O3P + NO2 = NO3 + M
	0:	9.00e-32	0.00	-2.0		
	inf:	2.20e-11	0.00	0.0		
8	1.87e-14	1.80e-12	2.72		6	O3 + NO = NO2 + O2
9	3.72e-17	1.40e-13	4.91		6	O3 + NO2 = O2 + NO3
10	2.60e-11	1.80e-11	-0.22		6	NO + NO3 = #2 NO2
11	1.93e-38	3.30e-39	-1.05		6	NO + NO + O2 = #2 NO2
12	1.53e-12	Falloff, F=0.45			6,7	NO2 + NO3 = N2O5
	0:	2.80e-30	0.00	-3.5		
	inf:	2.00e-12	0.00	0.2		
13	6.74e-2	Falloff, F=0.45			6,7	N2O5 = NO2 + NO3
	0:	1.00e-3	21.86	-3.5		
	inf:	9.70e+14	22.02	0.1		
14	2.60e-22	2.60e-22			9	N2O5 + H2O = #2 HNO3
15		(Slow)			10	N2O5 + HV = NO3 + NO + O3P
16		(Slow)			10	N2O5 + HV = NO3 + NO2
17	6.75e-16	4.50e-14	2.50		11	NO2 + NO3 = NO + NO2 + O2
18		Phot Set= NO3NO			1,12,13	NO3 + HV = NO + O2
19		Phot Set= NO3NO2			1,12,13	NO3 + HV = NO2 + O3P
20		Phot Set= O3O3P			1,14,15	O3 + HV = O3P + O2
21		Phot Set= O3O1D			1,14,15	O3 + HV = O*1D2 + O2
22	2.20e-10	2.20e-10			4	O*1D2 + H2O = #2 HO.
23	2.87e-11	2.09e-11	-0.19		16	O*1D2 + M = O3P + M
24	7.31e-12	Falloff, F=0.60			17	HO. + NO = HONO
	0:	7.00e-31	0.00	-2.6		
	inf:	3.60e-11	0.00	-0.1		
25		Phot Set= HONO-NO			1,18,19	HONO + HV = HO. + NO
26		Phot Set= HONO-NO2			1,18,19	HONO + HV = HO2. + NO2
27	6.42e-12	2.70e-12	-0.52		6	HO. + HONO = H2O + NO2
28	8.81e-12	Falloff, F=0.60			20	HO. + NO2 = HNO3
	0:	2.43e-30	0.00	-3.1		
	inf:	1.67e-11	0.00	-2.1		
29	2.00e-11	2.00e-11			6,21	HO. + NO3 = HO2. + NO2
30	1.44e-13	5.45e-15	-1.95		23,22	HO. + HNO3 = H2O + NO3
31		Phot Set= HNO3			1,24	HNO3 + HV = HO. + NO2
32A	1.30e-13	1.30e-13			25	HO. + CO = HO2. + CO2
32B	3.19e-33	3.19e-33			25	HO. + CO + M = HO2. + CO2 + M
33	6.78e-14	1.90e-12	1.99		6	HO. + O3 = HO2. + O2
34	8.36e-12	3.40e-12	-0.54		6	HO2. + NO = HO. + NO2
35	1.36e-12	Falloff, F=0.60			6	HO2. + NO2 = HNO4
	0:	1.80e-31	0.00	-3.2		
	inf:	4.70e-12	0.00	0.0		

SAPRC-99 Base Mechanism as of 1/9/99

Label	Rate Parameters [a]				Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea	B		
36	9.61e-2	Falloff, F=0.50			6	HNO4 = HO2. + NO2
	0:	4.10e-5	21.16	0.0		
	inf:	5.70e+15	22.20	0.0		
37	Phot Set= HO2NO2				1,26	HNO4 + HV = #.61 {HO2. + NO2} + #.39 {HO. + NO3}
38	4.98e-12	1.50e-12	-0.72		6	HNO4 + HO. = H2O + NO2 + O2
39	1.89e-15	1.40e-14	1.19		6	HO2. + O3 = HO. + #2 O2
40A	1.63e-12	2.20e-13	-1.19		27	HO2. + HO2. = HO2H + O2
40B	3.48e-30	3.08e-34	-5.56		27	HO2. + HO2. + H2O = HO2H + O2 + H2O
40C	4.85e-32	1.85e-33	-1.95		27	HO2. + HO2. + M = HO2H + O2 + M
40D	1.04e-49	2.59e-54	-6.32		27	HO2. + HO2. + M + H2O = HO2H + O2 + M + H2O
41	4.00e-12	4.00e-12			28	NO3 + HO2. = HO. + NO2 + O2
42	2.41e-16	8.50e-13	4.87		29	NO3 + NO3 = #2 NO2 + O2
43	Phot Set= H2O2				1,30	HO2H + HV = #2 HO.
44	1.70e-12	2.90e-12	0.32		6	HO2H + HO. = HO2. + H2O
45	1.10e-10	4.80e-11	-0.50		6	HO. + HO2. = H2O + O2
Methyl peroxy and methoxy reactions						
MER1	7.24e-12	2.80e-12	-0.57		31,32	C-O2. + NO = NO2 + C-O.
MER4	5.12e-12	3.80e-13	-1.55		31	C-O2. + HO2. = COOH + O2
MEN3	1.30e-12	1.30e-12			31	C-O2. + NO3 = C-O. + NO2 + O2
MER5	2.61e-13	2.45e-14	-1.41		35	C-O2. + C-O2. = MEOH + HCHO + O2
MER6	1.08e-13	5.90e-13	1.01		35	C-O2. + C-O2. = #2 C-O. + O2
MER7	1.97e-15	7.20e-14	2.15		31	C-O. + O2 = HCHO + HO2.
MER8	1.61e-11	Falloff, F=0.44			8,31	C-O. + NO2 = CONO2
	0:	9.00e-29	0.00	-4.5		
	inf:	1.90e-11	0.00	0.0		
Reactions of PAN and Acetyl Peroxy Radicals						
APN2	1.04e-11	Falloff, F=0.30			36	CCO-O2. + NO2 = PAN
	0:	2.70e-28	0.00	-7.1		
	inf:	1.20e-11	0.00	-0.9		
DPAN	7.04e-4	Falloff, F=0.30			37	PAN = CCO-O2. + NO2
	0:	4.90e-3	24.05	0.0		
	inf:	4.00e+16	27.03	0.0		
APNO	2.18e-11	2.18e-11			38	CCO-O2. + NO = C-O2. + CO2 + NO2
APH2	1.38e-11	4.30e-13	-2.07		39	CCO-O2. + HO2. = #.75 {CCO-OOH + O2} + #.25 {CCO-OH + O3}
APN3	4.00e-12	4.00e-12			39a	CCO-O2. + NO3 = C-O2. + CO2 + NO2 + O2
APME	9.53e-12	1.80e-12	-0.99		39b	CCO-O2. + C-O2. = CCO-OH + HCHO + O2
APAP	1.54e-11	2.90e-12	-0.99		31	CCO-O2. + CCO-O2. = #2 {C-O2. + CO2} + O2
Total Peroxy Radical Species						
LPNO	8.96e-12	2.70e-12	-0.72		40,41,32	RO2. + NO = NO
LPH2	1.45e-11	1.90e-13	-2.58		40,41	RO2. + HO2. = HO2.
LPN3	2.30e-12	2.30e-12			40,42	RO2. + NO3 = NO3
LPME	2.00e-13	2.00e-13			40,43	RO2. + C-O2. = C-O2.

SAPRC-99 Base Mechanism as of 1/9/99

Label	Rate Parameters [a]				Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea	B		
LPAP	1.00e-11	1.00e-11			40,44	RO2. + CCO-O2. = CCO-O2.
LPP2	1.00e-11	1.00e-11			40,44	RO2. + RCO3. =
LPR2	3.00e-14	3.00e-14			40,45	RO2. + RO2. =
Total Acyl Peroxy Radical Species						
LAN2	1.20e-11	1.20e-11	0.00	-0.9	40,46	RCO3. + NO2 = NO2
LANO	Same k as rxn APNO				40,47	RCO3. + NO = NO
LAH2	Same k as rxn APH2				40,47	RCO3. + HO2. = HO2.
LAN3	Same k as rxn APN3				40,47	RCO3. + NO3 = NO3
LAME	Same k as rxn APME				40,47	RCO3. + C-O2. = C-O2.
LAAP	Same k as rxn APAP				40,47	RCO3. + CCO-O2. = CCO-O2.
LALA	Same k as rxn APAP				40,47	RCO3. + RCO3. =
Peroxy Racical Operators						
R2XX	(Fast)				48	R2O2. = [R2O2] + RO2.
R2NO	Same k as rxn LPNO				50,49	[R2O2] + NO = NO2
R2H2	Same k as rxn LPH2				50,49	[R2O2] + HO2. = HO2.
R2ME	Same k as rxn LPME				50,49	[R2O2] + C-O2. = C-O2.
R2N3	Same k as rxn LPN3				50,49	[R2O2] + NO3 = NO2
R2AP	Same k as rxn LPAP				50,49	[R2O2] + CCO-O2. = CCO-O2.
R2P2	Same k as rxn LPP2				50,49	[R2O2] + RCO3. = RCO3.
R2R2	Same k as rxn LPR2				50,49	[R2O2] + RO2. = RO2.
RRXX	(Fast)				48	RO2-R. = [RO2-R] + RO2.
RRNO	Same k as rxn LPNO				51,49	[RO2-R] + NO = NO2 + HO2.
RRH2	Same k as rxn LPH2				51,49,52	[RO2-R] + HO2. = ROOH + O2 + #-3 XC
RRME	Same k as rxn LPME				51,49,53	[RO2-R] + C-O2. = #.5 {C-O. + HO2.} + #.25 {HCHO + MEOH}
RRN3	Same k as rxn LPN3				51,49,54	[RO2-R] + NO3 = NO2 + O2 + HO2.
RRAP	Same k as rxn LPAP				51,49,54a	[RO2-R] + CCO-O2. = CCO-OH
RRP2	Same k as rxn LPP2				51,49,53	[RO2-R] + RCO3. = RCO3. + #.5 HO2.
RRR2	Same k as rxn LPR2				51,49,53	[RO2-R] + RO2. = RO2. + #.5 HO2.
RNXX	(Fast)				48	RO2-N. = [RO2-N] + RO2.
RNNO	Same k as rxn LPNO				55,49	[RO2-N] + NO = RNO3
RNH2	Same k as rxn LPH2				55,49,56	[RO2-N] + HO2. = ROOH + #2 XC
RNME	Same k as rxn LPME				55,49,57	[RO2-N] + C-O2. = #.5 {C-O. + MEK + HO2.} + #.25 {HCHO + MEOH + MEK + PROD2} + O2 + #1.25 XC
RNN3	Same k as rxn LPN3				55,49,58	[RO2-N] + NO3 = NO2 + O2 + HO2. + MEK + XC
RNAP	Same k as rxn LPAP				55,49, 54a,58a	[RO2-N] + CCO-O2. = CCO-OH + PROD2
RNP2	Same k as rxn LPP2				55,49,57	[RO2-N] + RCO3. = RCO3. + MEK + #.5 HO2. + XC
RNR2	Same k as rxn LPR2				55,49,57	[RO2-N] + RO2. = RO2. + #.5 {MEK + HO2. + PROD2} + O2 + #1.5 XC
RXXX	(Fast)				48	RO2-XN. = [RO2-XN] + RO2.
RXNO	Same k as rxn LPNO				59,49	[RO2-XN] + NO = XN
RXH2	Same k as rxn LPH2				59,49,52	[RO2-XN] + HO2. = ROOH + #-3 XC
RXME	Same k as rxn LPME				59,49,53	[RO2-XN] + C-O2. = #.5 C-O. + #.25 {HCHO + MEOH}

SAPRC-99 Base Mechanism as of 1/9/99

Label	Rate Parameters [a]			Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea B		
RXN3		Same k as rxn LPN3		59,49,54	[RO2-XN] + NO3 = NO2 + O2 + HO2.
RXAP		Same k as rxn LPAP		59,49,54a	[RO2-XN] + CCO-O2. = CCO-OH
RXP2		Same k as rxn LPP2		59,49,53	[RO2-XN] + RCO3. = RCO3.
RXR2		Same k as rxn LPR2		59,49,53	[RO2-XN] + RO2. = RO2.
RPXX		(Fast)		48	RO2-NP. = [RO2-NP] + RO2.
RPNO		Same k as rxn LPNO		60,49	[RO2-NP] + NO = NPHE
RPH2		Same k as rxn LPH2		60,49,61	[RO2-NP] + HO2. = PHEN
RPME		Same k as rxn LPME		60,49,62	[RO2-NP] + C-O2. = #.5 {C-O. + BZ-O. + HCHO + PHEN}
RPN3		Same k as rxn LPN3		60,49,63	[RO2-NP] + NO3 = NO2 + BZ-O.
RPAP		Same k as rxn LPAP		60,49,63	[RO2-NP] + CCO-O2. = C-O2. + CO2 + BZ-O.
RPP2		Same k as rxn LPP2		60,49,63	[RO2-NP] + RCO3. = RCO3. + BZ-O.
RPR2		Same k as rxn LPR2		60,49,62	[RO2-NP] + RO2. = RO2. + #.5 {BZ-O. + PHEN}
Lumped and Miscellaneous Acyl Peroxy Radicals and PAN Analogues					
PPXX		(Fast)		48	RCO-O2. = [RCO-O2] + RCO3.
PPN2		Same k as rxn LAN2		64,65	[RCO-O2] + NO2 = PAN2
PPNO		Same k as rxn APNO		64,65	[RCO-O2] + NO = NO2 + CCHO + RO2-R. + CO2
PPH2		Same k as rxn APH2		64,65	[RCO-O2] + HO2. = RCO-OOH + O2
PPN3		Same k as rxn APN3		64,65	[RCO-O2] + NO3 = NO2 + CCHO + RO2-R. + CO3 + O2
PPME		Same k as rxn APME		64,65	[RCO-O2] + C-O2. = RCO-OH + HCHO + O2
PPAP		Same k as rxn APAP		64,65	[RCO-O2] + CCO-O2. = #2 CO2 + C-O2. + CCHO + RO2-R. + O2
PPR2		Same k as rxn LPAP		64,65	[RCO-O2] + RO2. = RO2. + RCO-OH
PPLA		Same k as rxn APAP		64,65	[RCO-O2] + RCO3. = RCO3. + CCHO + RO2-R. + CO2
PAN2	5.87e-4	2.00e+15	25.44	65,66	PAN2 = RCO-O2. + NO2
GPXX		(Fast)		48	HCOCO-O2. = [HCOCO-O2] + RCO3.
GPN2		Same k as rxn LAN2		64	[HCOCO-O2] + NO2 = GPAN
GPNO		Same k as rxn APNO		64	[HCOCO-O2] + NO = NO2 + CO2 + CO + HO2.
GPH2		Same k as rxn APH2		64	[HCOCO-O2] + HO2. = RCO-OOH + O2
GPN3		Same k as rxn APN3		64	[HCOCO-O2] + NO3 = NO2 + CO2 + CO + HO2. + O2
GPME		Same k as rxn APME		64	[HCOCO-O2] + C-O2. = RCO-OH + HCHO + O2
GPAP		Same k as rxn APAP		64	[HCOCO-O2] + CCO-O2. = #2 CO2 + C-O2. + HO2. + CO + O2
GPR2		Same k as rxn LPAP		64	[HCOCO-O2] + RO2. = RO2. + #.5 {RCO-OH + HO2. + CO + CO2}
GPLA		Same k as rxn APAP		64	[HCOCO-O2] + RCO3. = RCO3. + HO2. + CO + CO2
GPAN		Same k as rxn PAN2		64	GPAN = HCOCO-O2. + NO2
BPXX		(Fast)		48	BZCO-O2. = [BZCO-O2] + RCO3.

SAPRC-99 Base Mechanism as of 1/9/99

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	k(300)	A	Ea	B		
BPN2	1.37e-11	1.37e-11			67	[BZCO-O2] + NO2 = PBZN
BPNO		Same k as rxn APNO			64	[BZCO-O2] + NO = NO2 + CO2 + BZ-O. + R2O2.
BPH2		Same k as rxn APH2			64	[BZCO-O2] + HO2. = RCO-OOH + O2
BPNO3		Same k as rxn APN3			64	[BZCO-O2] + NO3 = NO2 + CO2 + BZ-O. + R2O2. + O2
BPME		Same k as rxn APME			64	[BZCO-O2] + C-O2. = RCO-OH + HCHO + O2
BPAP		Same k as rxn APAP			64	[BZCO-O2] + CCO-O2. = #2 CO2 + C-O2. + BZ-O. + R2O2.
BPR2		Same k as rxn LPAP			64	[BZCO-O2] + RO2. = RO2. + #.5 {RCO-OH + BZ-O. + R2O2. + CO2}
BPLA		Same k as rxn APAP			64	[BZCO-O2] + RCO3. = RCO3. + BZ-O. + R2O2. + CO2
BPAN	4.27e-4	7.90e+16	27.82		68	PBZN = BZCO-O2. + NO2
MPXX			(Fast)		48	MA-RCO3. = [MA-RCO3] + RCO3.
MPN2		Same k as rxn LAN2			69,64	[MA-RCO3] + NO2 = MA-PAN
MPNO		Same k as rxn APNO			69,64	[MA-RCO3] + NO = NO2 + CO2 + HCHO + CCO-O2.
MPH2		Same k as rxn APH2			69,64	[MA-RCO3] + HO2. = RCO-OOH + O2 + XC
MPN3		Same k as rxn APN3			69,64	[MA-RCO3] + NO3 = NO2 + CO2 + HCHO + CCO-O2. + O2
MPME		Same k as rxn APME			69,64	[MA-RCO3] + C-O2. = RCO-OH + HCHO + XC + O2
MPAP		Same k as rxn APAP			69,64	[MA-RCO3] + CCO-O2. = #2 CO2 + C-O2. + HCHO + CCO-O2. + O2
MPR2		Same k as rxn LPAP			69,64	[MA-RCO3] + RO2. = RO2. + RCO-OH + XC
MPLA		Same k as rxn APAP			69,64	[MA-RCO3] + RCO3. = RCO3. + HCHO + CCO-O2. + CO2
MPPN	4.79e-4	1.60e+16	26.80		70	MA-PAN = MA-RCO3. + NO2
Other Organic Radical Species						
TBON	2.40e-11	2.40e-11			71,72	TBU-O. + NO2 = RNO3 + #-2 XC
TBOD	1.18e+3	7.50e+14	16.20		73,72	TBU-O. = ACET + C-O2.
BRN2	3.79e-11	2.30e-11	-0.30		74	BZ-O. + NO2 = NPHE
BRH2		Same k as rxn LPH2			75	BZ-O. + HO2. = PHEN
BRXX	1.00e-3	1.00e-3			76	BZ-O. = PHEN
BNN2		Same k as rxn BRN2			77	BZ(NO2)-O. + NO2 = #2 XN + #6 XC
BNH2		Same k as rxn LPH2			75	BZ(NO2)-O. + HO2. = NPHE
BNXX		Same k as rxn BRXX			76	BZ(NO2)-O. = NPHE
Explicit Organic Products						
FAHV		Phot Set= HCHO_R			78	HCHO + HV = #2 HO2. + CO
FAVS		Phot Set= HCHO_M			78	HCHO + HV = H2 + CO
FAOH	9.19e-12	8.60e-12	-0.04		31	HCHO + HO. = HO2. + CO + H2O
FAH2	7.79e-14	9.70e-15	-1.24		31	HCHO + HO2. = HOCOO.
FAHR	1.76e+2	2.40e+12	13.91		31	HOCOO. = HO2. + HCHO
FAHN		Same k as rxn MER1			79	HOCOO. + NO = HCOOH + NO2 + HO2.

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Label	Rate Parameters [a]				Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea	B		
FAN3	6.06e-16	2.00e-12	4.83		80	HCHO + NO3 = HNO3 + HO2. + CO
MeOH	9.34e-13	3.10e-12	0.72	2.0	81	MEOH + HO. = #.85 HO2. + #.15 C-O. + #.85 HCHO
MER9	5.46e-12	2.90e-12	-0.38		82	COOH + HO. = H2O + #.35 {HCHO + HO.} + #.65 C-O2.
MERA		Phot Set= COOH			83	COOH + HV = C-O. + HO.
AAOH	1.57e-11	5.60e-12	-0.62		31	CCHO + HO. = CCO-O2. + H2O
AAHV		Phot Set= CCHO_R			84	CCHO + HV = CO + HO2. + C-O2.
AAN3	2.84e-15	1.40e-12	3.70		33	CCHO + NO3 = HNO3 + CCO-O2.
K3OH	1.94e-13	1.10e-12	1.03		31,85	ACET + HO. = HCHO + CCO-O2. + R2O2.
K3HV		Phot Set= ACETONE			86	ACET + HV = CCO-O2. + C-O2.
GLHV		Phot Set= GLY_R			87,88	GLY + HV = #2 {CO + HO2.}
GLVM		Phot Set= GLY_ABS, qy= 6.0e-3			87,89	GLY + HV = HCHO + CO
GLOH	1.10e-11	1.10e-11			31,90	GLY + HO. = #.63 HO2. + #1.26 CO + #.37 HCOCO-O2.
GLN3		Same k as rxn AAN3			91	GLY + NO3 = HNO3 + #.63 HO2. + #1.26 CO + #.37 HCOCO-O2.
MGHV		Phot Set= MGLY_ADJ			92	MGLY + HV = HO2. + CO + CCO-O2.
MGOH	1.50e-11	1.50e-11			31	MGLY + HO. = CO + CCO-O2.
MGN3		Same k as rxn AAN3			91	MGLY + NO3 = HNO3 + CO + CCO-O2.
BAHV		Phot Set= BACL_ADJ			87,93	BACL + HV = #2 CCO-O2.
ACOH	1.99e-11	1.99e-11			94,95,96, 97	ACROLEIN + HO. = #.25 RO2-R. + #.167 CO + #.083 HCHO + #.167 RCHO + #.083 GLY + #.75 MA-RCO3. + #-.917 XC
ACO3	3.05e-19	1.36e-15	5.01		98,99, 100,101	ACROLEIN + O3 = #.32 RO2-R. + #.32 HO. + #.77 CO + #.135 CO2 + #.57 HCHO + #.5 GLY + #.185 HCHO2-STAB + #.17 RCHO2-STAB + #-.017 XC
ACN3	1.05e-16	4.59e-13			102,103, 96,104	ACROLEIN + NO3 = #.964 RO2-R. + #.036 RO2-N. + #.964 CO + #.964 RCHO + #-.1036 XC + XN
ACOP	2.40e-12	2.40e-12			105,5	ACROLEIN + O3P = RCHO
ACHV		Phot Set= ACROLEIN, qy= 3.3e-3			106,107, 108,109, 96,97	ACROLEIN + HV = #1.01 HO2. + #.172 RO2-R. + #.172 HO. + #1.182 CO + #.046 CO2 + #.512 HCHO + #.33 MA-RCO3. + #-.284 XC + #.112 CCHO2-STAB + #.046 NROG
MAOH	3.35e-11	1.86e-11	-0.35		110,96, 111	METHACRO + HO. = #.5 RO2-R. + #.416 CO + #.084 HCHO + #.416 MEK + #.084 MGLY + #.5 MA-RCO3. + #-.0416 XC
MAO3	1.19e-18	1.36e-15	4.20		110,100, 112	METHACRO + O3 = #.008 HO2. + #.1 RO2-R. + #.208 HO. + #.1 RCO-O2. + #.45 CO + #.117 CO2 + #.2 HCHO + #.9 MGLY + #.333 HCHO2-STAB + #-.01 XC
MAN3	4.76e-15	1.50e-12	3.43		110,103, 96,113	METHACRO + NO3 = #.5 {HNO3 + RO2-R. + CO + MA-RCO3.} + #1.5 XC + #.5 XN
MAOP	6.34e-12	6.34e-12			105,5	METHACRO + O3P = RCHO + XC

SAPRC-99 Base Mechanism as of 1/9/99

Label	Rate Parameters [a]				Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea	B		
MAHV	Phot Set= ACROLEIN, qy= 4.1e-3				110,114	METHACRO + HV = #.34 HO2. + #.33 RO2-R. + #.33 HO. + #.67 CCO-O2. + #.67 CO + #.67 HCHO + #.33 MA-RCO3. + #0 XC
MVOH	1.87e-11	4.14e-12	-0.90		110,96	MVK + HO. = #.3 RO2-R. + #.025 RO2-N. + #.675 R2O2. + #.675 CCO-O2. + #.3 HCHO + #.675 RCHO + #.3 MGLY + #0.7 XC
MVO3	4.74e-18	7.51e-16	3.02		110,100, 112,96	MVK + O3 = #.064 HO2. + #.05 RO2-R. + #.164 HO. + #.05 RCO-O2. + #.475 CO + #.124 CO2 + #.1 HCHO + #.95 MGLY + #.351 HCHO2-STAB + #0.05 XC
MVN3		(Slow)			110	MVK + NO3 = products
MVOP	4.32e-12	4.32e-12			105,5	MVK + O3P = #.45 RCHO + #.55 MEK + #.45 XC
MVHV	Phot Set= ACROLEIN, qy= 2.1e-3				110,114, 97	MVK + HV = #.3 RO2-R. + #.7 CO + #.3 HCHO + #.7 PROD2 + #.3 MA-RCO3. + #2.4 XC
PHOH	2.63e-11	2.63e-11			116,117	PHEN + HO. = #.24 BZ-O. + #.76 RO2-R. + #.23 GLY + #4.1 XC
PHN3	3.78e-12	3.78e-12			116,118	PHEN + NO3 = HNO3 + BZ-O.
Lumped Organic Products						
LPR9	1.10e-11	1.10e-11			120,121	ROOH + HO. = H2O + RCHO + #.34 RO2-R. + #.66 HO.
LPRA	Phot Set= COOH				122	ROOH + HV = RCHO + HO2. + HO.
PAOH	2.00e-11	2.00e-11			123, 31, 124,96	RCHO + HO. = #.034 RO2-R. + #.001 RO2-N. + #.965 RCO-O2. + #.034 CO + #.034 CCHO + #0.003 XC
PAHV	Phot Set= C2CHO				123,84	RCHO + HV = CCHO + RO2-R. + CO + HO2.
PAN3	Same k as rxn AAN3				123,125	RCHO + NO3 = HNO3 + RCO-O2.
K4OH	1.20e-12	1.30e-12	0.05	2.0	31,124,96	MEK + HO. = #.374 RO2-R. + #.042 RO2-N. + #.609 R2O2. + #.491 CCO-O2. + #.093 RCO-O2. + #.109 HCHO + #.483 CCHO + #.374 RCHO + #.332 XC
K4HV	Phot Set= KETONE, qy= 1.0e-1				126	MEK + HV + #QY.MEK = CCO-O2. + CCHO + RO2-R.
RNOH	2.99e-12	2.99e-12			127,128, 124,96, 129	RNO3 + HO. = #.505 RO2-R. + #.111 RO2-N. + #.708 R2O2. + #.004 HCHO + #.393 CCHO + #.455 RCHO + #.032 MEK + #.034 PROD2 + #.136 XC + #.251 XN + #.365 RNO3 + #.384 NO2
RNHV	Phot Set= IC3ONO2				127,130, 96	RNO3 + HV = #.868 RO2-R. + #.132 HO2. + #.031 CCHO + #.031 RCHO + #.132 MEK + #.838 PROD2 + #0.706 XC + NO2
K6OH	9.64e-12	9.64e-12			131,128, 124,96, 132	PROD2 + HO. = #.521 RO2-R. + #.044 RO2-N. + #.342 HO2. + #.082 CCO-O2. + #.011 RCO-O2. + #.439 HCHO + #.945 RCHO + #1.308 XC

SAPRC-99 Base Mechanism as of 1/9/99

Label	Rate Parameters [a]			Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea B		
K6HV		Phot Set= KETONE		131,133, 96	PROD2 + HV + #QY.K6 = RO2-R. + #.015 R2O2. + CCO-O2. + #.038 HCHO + #.988 RCHO + #-0.003 XC
CROH	4.20e-11	4.20e-11		116,134	CRES + HO. = #.24 BZ-O. + #.76 RO2-R. + #.23 MGLY + #4.87 XC
CRN3	1.37e-11	1.37e-11		116,118	CRES + NO3 = HNO3 + BZ-O. + XC
BZOH	1.29e-11	1.29e-11		116	BALD + HO. = BZCO-O2.
BZHV		Phot Set= BZCHO, qy= 5.0e-2		135	BALD + HV = #7 XC
BZNT	2.73e-15	1.40e-12	3.72	136	BALD + NO3 = HNO3 + BZCO-O2.
NPN3	S		0.00	137	NPHE + NO3 = HNO3 + BZ(NO2)-O.
D1OH	5.00e-11	5.00e-11		138,139	DCB1 + HO. = RCHO + RO2-R. + CO
D1HV		Phot Set= ACROLEIN, qy= 3.4e-3		138,140	DCB1 + HV = HO2. + #2 CO + RO2-R. + GLY + R2O2.
D1O3	2.00e-18	2.00e-18		138,141, 101	DCB1 + O3 = #.52 RO2-R. + #.52 HO. + #1.04 CO + #.14 CO2 + #.14 HCHO + GLY + #.34 RCHO2-STAB + #-0.34 XC
D2OH	5.00e-11	5.00e-11		142,143	DCB2 + HO. = R2O2. + RCHO + CCO-O2.
D3OH	5.00e-11	5.00e-11		142,143	DCB3 + HO. = R2O2. + RCHO + CCO-O2.
D2HV		Phot Set= MGLY_ABS, qy= 3.7e-1		142,144	DCB2 + HV + #D2HV = RO2-R. + #.5 {CCO-O2. + HO2.} + CO + R2O2. + #.5 {GLY + MGLY + XC}
D3HV		Phot Set= ACROLEIN, qy= 7.3e+0		142,144	DCB3 + HV + #D3HV = RO2-R. + #.5 {CCO-O2. + HO2.} + CO + R2O2. + #.5 {GLY + MGLY + XC}
D4OH	5.00e-11	5.00e-11		145,146	DCB4 + HO. = RCHO + RO2-R. + CO + #2 XC
D4O3	2.00e-18	2.00e-18		145,147, 112	DCB4 + O3 = R2O2. + HO. + RCO-O2. + HCHO + MGLY + #-1 XC
IPOH	6.19e-11	6.19e-11		148,110, 96	ISOPROD + HO. = #.705 RO2-R. + #.006 RO2-N. + #.357 CO + #.056 HCHO + #.148 RCHO + #.159 MEK + #.353 PROD2 + #.159 GLY + #.179 MGLY + #.289 MA-RCO3. + #-949 XC
IPO3	4.18e-18	4.18e-18		148,110, 96,101, 112,149	ISOPROD + O3 = #.132 HO2. + #.11 RO2-R. + #.289 HO. + #.048 RCO-O2. + #.402 CO + #.065 CO2 + #.155 HCHO + #.047 RCHO + #.211 MEK + #.023 GLY + #.742 MGLY + #.1 HCHO2-STAB + #.443 RCHO2-STAB + #-748 XC
IPN3	1.00e-13	1.00e-13		148,110, 96	ISOPROD + NO3 = #.15 HNO3 + #.85 RO2-R. + #.608 CO + #.242 HCHO + #.234 RCHO + #.608 RNO3 + #.008 MGLY + #.15 MA-RCO3. + #-517 XC + #.242 XN
IPHV		Phot Set= ACROLEIN, qy= 4.1e-3		148,110, 96, 150	ISOPROD + HV = #1.234 RO2-R. + #.466 CCO-O2. + #.3 RCO-O2. + #1.234 CO + #.3 HCHO + #.466 RCHO + #.234 MEK + #-1 XC

Explicit Primary Organics

SAPRC-99 Base Mechanism as of 1/9/99

Label	Rate Parameters [a]				Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea	B		
c1OH	6.62e-15	2.15e-12	3.45		31	CH4 + HO. = H2O + C-O2.
ISOH	9.73e-11	2.50e-11	-0.81		151,152	ISOPRENE + HO. = #.909 RO2-R. + #.091 RO2-N. + #.079 R2O2. + #.626 HCHO + #.23 METHACRO + #.32 MVK + #.359 ISOPROD + #-.076 XC
ISO3	1.34e-17	7.86e-15	3.80		151,100, 153	ISOPRENE + O3 = #.066 RO2-R. + #.134 R2O2. + #.266 HO. + #.275 CO + #.122 CO2 + #.6 HCHO + #.1 PROD2 + #.39 METHACRO + #.16 MVK + #.2 MA-RCO3. + #.204 HCHO2-STAB + #.15 RCHO2-STAB + #-.025 XC
ISN3	6.81e-13	3.03e-12	0.89		151, 154	ISOPRENE + NO3 = #.19 NO2 + #.76 RO2-R. + #.05 RO2-N. + #.19 R2O2. + #.95 ISOPROD + #.81 XN
ISOP	3.60e-11	3.60e-11			151, 155	ISOPRENE + O3P = #.25 RO2-R. + #.25 R2O2. + #.5 HCHO + #.75 PROD2 + #.25 MA-RCO3. + #-1 XC

Documentation Notes

No.	Note
1	See Table ?? for listing of absorption cross sections and quantum yields. Set used is given in the "Type" column.
2	Absorption cross sections and quantum yields from IUPAC recommendation (Atkinson et al, 1997a), except that quantum yields for $\lambda > 410$ nm are from NASA (1997), which are consistent with IUPAC (Atkinson et al, 1997a) values except they are more precise. Note that more recent IUPAC recommendations (Atkinson et al, 1997b) gives slightly different absorption cross sections based on data from a more recent study, but the differences are not significant.
3	Rate constant expression derived from IUPAC (Atkinson et al, 1997b) recommendations for M = 20.9% O ₂ and 79.1% N ₂ .
4	Rate constant is IUPAC, Supplement VI (Atkinson et al, 1997b) and NASA (1997) recommendation.
5	This reaction is probably not important in air, but is included to increase range of applicability.
6	Rate constant expression is IUPAC (Atkinson et al, 1997b) recommendation.
7	Recommended rate constant given for N ₂ is assumed to be applicable to air.
8	(note deleted)
9	The data of Mentel et al (1996) indicate that the reaction occurs through pathways which are first order and second order in H ₂ O, where the latter is presumed to be surface-dependent. We assume that the process which is first order in H ₂ O represents a gas-phase reaction, and use the rate expression of Mentel et al (1996) for this process. Note that this is inconsistent with the IUPAC (Atkinson et al, 1997b) recommendation that the gas-phase rate constant is less than 2×10^{-21} cm ³ molec ⁻¹ s ⁻¹ .
10	Photolysis of N ₂ O ₅ is assumed to be negligible compare to decomposition under atmospheric conditions.
11	The NASA (1997) evaluation states that the existence of this channel has not been firmly established, but results of a number of studies indicate it may occur. Rate constant expression used is that NASA (1997) states gives best fits to the data. Uncertainty is at least a factor of 2. This reaction was not discussed in the recent IUPAC evaluations (Atkinson et al, 1997a,b).
12	Absorption cross sections from IUPAC (Atkinson et al, 1997a). Values recommended by more recent IUPAC evaluation (Atkinson et al, 1997b) appear to be the same for 298K, though different at lower temperature. Temperature dependence ignored.
13	IUPAC (1997b) and NASA (1997) give no useable recommendations for quantum yields except to recommend that $q(\text{NO}_2+\text{O})=1$ for $\lambda \leq 583$. Quantum yields of Magnotta and Johnson (1980), scaled down by a factor of 1.5 to give unit maximum quantum yields, as incorporated in mechanism of Carter (1990) were retained in this mechanism. The calculated rate constant for solar overhead sun is consistent with the recommendations of Magnotta and Johnson (1980), and reasonably consistent with the IUPAC (1997a) recommendation.
14	Absorption cross sections from IUPAC (Atkinson et al, 1997b). Data are for T=273 K. Temperature dependences for cross section (NASA, 1997) are ignored.
15	Quantum yields for O ¹ D are those tabulated by IUPAC (Atkinson et al, 1997b), which are significantly higher than previous recommendations at $\lambda > 310$ nm. Quantum yields for O ³ P based on assuming total quantum yield of unity, though this was not adequately discussed in the evaluations.
16	Calculated using IUPAC (Atkinson et al, 1997b) recommended rate constants for reaction with O ₂ and N ₂ , assuming 20.9% O ₂ and 79.1% N ₂ . Temperature dependence optimized to fit rate constants calculated for T= 270, 300, and 330K.
17	Falloff expression recommended by NASA (1997) used because it gives rate constant for 1 atm N ₂ which is consistent with measurement near those conditions. IUPAC (Atkinson et al, 1997a,b) recommendations are not used because k (1 atm N ₂) are not consistent with these data, being based on high pressure data in He. This is consistent with current recommendation of Atkinson (private communication, 1997).

Documentation Notes

No.	Note
18	The cross sections from Stockwell and Calvert (1978), used in the previous version of the mechanism, are retained because they are higher resolution than the averaged data recommended by IUPAC (1997b), and the areas under the spectra appear to be consistent.
19	Quantum yields are those recommended by IUPAC (Atkinson et al, 1997b).
20	NASA (1997) and IUPAC (Atkinson et al, 1997a,b) give significantly different recommendations for rate parameters for this important reaction. The falloff expression used here is based on a NASA (1997) and IUPAC (Atkinson et al, 1997a,b) give significantly different recommendations for rate parameters for this important reaction. The falloff expression used here is based on a re-evaluation of the data by Golden (Personal communication, 1998), and is expected to be the recommendation in the next NASA evaluation. This is essentially the same as the NASA (1997) recommendation except for the temperature dependence, which Golden says was due to improper uncertainty weighting. The data with "weak colliders (i.e., bath gases other than SF ₆ or CF ₄) appear to be well fit by this parameterization, including the data of Donahue et al (1997). The data of Forster et al (1995), which are the basis for the high 1997 IUPAC recommendation, are not used because they may be due to a HOONO-forming channel becoming important at high pressure.
21	No recommendation is given concerning the temperature dependence of this rate constant, which is assumed to be small.
22	This rate constant is strictly valid for 1 atm air only, but the error introduced by neglecting the pressure dependence of this reaction is expected to be small.
23	The rate parameters were derived to fit the rate constants calculated using the NASA (1997) recommended expression for T 270 - 330 K range and 1 atm. total pressure.
24	Absorption cross-sections from IUPAC (Atkinson et al, 1997b). Recommend quantum yield for the OH + NO ₂ pathway is "close to unity" for $\lambda > 260$ nm, though other pathways become important at lower wavelengths.
25	The rate constants for the OH + CO reactions are based on expression given by IUPAC (Atkinson et al, 1997a). NASA (1997) gives a similar expression, but without temperature dependence.
26	Absorption cross sections and quantum yields from IUPAC (Atkinson et al, 1997b). Quantum yields are uncertain and based on data for a single wavelength only.
27	Reactions and rate constants used for the HO ₂ + HO ₂ and HO ₂ + HO ₂ + H ₂ O system based on the data of Kircher and Sander (1984) as discussed in the IUPAC (Atkinson et al, 1997b) evaluation.
28	Rate constant recommended by IUPAC (Atkinson et al, 1997b). Mechanism based on data of Mellouki et al (1993) as discussed by IUPAC (Atkinson et al, 1997b).
29	Rate expression from NASA (1994) evaluation. More recent evaluations neglect this reaction, though it may be non-negligible under some nighttime conditions (Stockwell et al, 1997).
30	Absorption cross sections recommended by IUPAC (Atkinson et al, 1997a,b) used. Quantum yield assumed to be unity.
31	Rate constant expression recommended by IUPAC, Supplement VII (Atkinson et al, 1999).
32	The reaction of NO ₂ is ignored because it is rapidly reversed by the decomposition of the peroxyxynitrate, resulting in no net reaction. Calculations not neglecting peroxyxynitrate formation give essentially the same results. However, this may not be valid in low temperature simulations.
33	Rate constant expression recommended by IUPAC, Supplement V (Atkinson et al, 1997a).
34	(note deleted)
35	Total rate constant and rate constant for methoxy radical formation from IUPAC (Atkinson et al, 1997a, 1999) recommendation. Temperature dependence for rate constant for methanol + HCHO formation derived to be consistent with these.
36	Falloff expression recommended by IUPAC (Atkinson et al, 1997a, 1999), based on data of Bridier et al (1991).

Documentation Notes

No.	Note
37	Falloff expression recommended by IUPAC (Atkinson et al, 1992), based on data of Bridier et al (1991). Note: NASA (1997) also recommends using Bridier et al (1991) data, but gives a revised expression which gives a different k at 298K. Based on new data on PAN decomposition which give a factor of ~2 lower rate 298K rate constants, IUPAC (1997a, 1999) recommends the a high pressure rate constant expression of $5.4 \times 10^{16} \exp(-13830/T)$, derived by averaging the data. We are staying with the earlier IUPAC Recommendations based on the data of Bridier et al (1991) because it gives good agreement with the data of Tuazon et al (1991) and is consistent with the NASA (1997) recommended equilibrium constant.
38	Rate constant based on the IUPAC (Atkinson et al, 1997a) recommendation is to use $k(\text{NO})/k(\text{NO}_2)=2.1$ for atmospheric conditions (298K and 1 atm.), with k(NO) approximately independent of temperature. This is almost the same as the IUPAC(Atkinson et al, 1997a, 1999) recommended value of 2.0×10^{-11} and the NASA (1997) value of 1.8×10^{-11} .
39	Branching ratio and rate constant expression recommended by IUPAC (Atkinson et al, 1997a, 1999).
39a	Rate constant from Canosa-Mass et al (1996)
39b	Rate constant expression recommended by IUPAC (Atkinson et al, 1999) evaluation. As discussed there, the data are inconclusive as to the importance of the competing reaction forming $\text{CH}_3\text{O} + \text{CH}_3\text{CO}_2 + \text{O}_2$, but the study which indicate that it occurs, which was used in the previous IUPAC (Atkinson et al, 1997a) evaluation, indicates that it occurs less than ~15% under atmospheric conditions.
40	Note that the purpose of this reaction is to compute the consumption rate of the total of all higher peroxy radicals, not the effect of peroxy radical reactions on other species, The latter are handled by reactions of the other peroxy radical operators.
41	Rate constant recommended by Atkinson (1997a) for general peroxy radicals.
42	Rate constant based on that recommended by IUPAC (Atkinson et al, 1999) for ethyl peroxy + NO ₂ . Formation of alkoxy + NO ₂ + O ₂ stated to occur >85% of the time.
43	Based on rate constant for methyl peroxy + ethyl peroxy rate given by Atkinson (1997a). This is near the middle of the range of rate constants given for other methyl peroxy + higher alkyl peroxy radical reactions given by Atkinson (1997a) or Atkinson et al (1997a).
44	Rate constant based on values for rate constants for acetyl peroxy + methyl peroxy and $\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{OO}$. given by Atkinson et al (1997a).
45	The rate constants for peroxy + peroxy radical reactions can vary by orders of magnitude depending on the type of radical (e.g., Atkinson, 1997), so the value used here must be approximate. Value used is based roughly on range of rate constants for secondary peroxy radicals as given by Atkinson (1997a).
46	The rate parameters are assumed to be approximately the same as those for the reaction of $\text{CH}_3\text{C}(\text{O})\text{OO}$. at the high pressure limit. NASA (1997) and IUPAC (Atkinson et al, 1997a, 1999) give no recommendations for this rate constant for higher acyl peroxy radicals.
47	Assumed to have same rate constant as corresponding reaction of $\text{CH}_3\text{C}(\text{O})\text{OO}$.
48	This fast pseudo-reaction, and the added [radical] operator, are included so that any reaction forming this peroxy radical operator will also form the total peroxy radical (RO ₂) species. The actual reactions of this operator are those shown below.
49	Assumed to have same rate constant as used for general higher peroxy radical.
50	This operator represents the effects of peroxy radical reactions causing extra NO to NO ₂ conversions. Its reactions with species other than NO are represented as having no effect other than to consume this operator.

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No.	Note
51	This operator represents the effects of peroxy radicals which react with NO to form NO ₂ and HO ₂ , and also the effects of peroxy radical reactions on other species. Except as indicated, the organic products from this peroxy radical are not represented.
52	The organic products from the HO ₂ reaction are represented by the lumped higher hydroperoxide species. Negative "lost carbons" are added because this is a zero-carbon operator.
53	Approximately half of the peroxy + peroxy reaction is assumed to form two O ₂ + alkoxy radicals. The 0.5 HO ₂ represents the radicals regenerated in the fraction of this peroxy radical which reacts in this way.
54	The reaction is assumed to form the corresponding alkoxy radical. The HO ₂ represents the radicals regenerated by the alkoxy radical.
54a	This reaction is assumed to proceed primarily by disproportionation to form the organic acid and a carbonyl compound, based on data for the acetyl peroxy + methyl peroxy reaction.
55	This operator represents the effects of peroxy radicals which react with NO to form higher organic nitrates (represented by RNO ₃), and also the effects of peroxy radical reactions on other species. It has five carbons.
56	The organic products from the HO ₂ reaction are represented by the lumped higher hydroperoxide species. "Lost carbons" are added because this is a five-carbon operator.
57	Approximately half of the peroxy + peroxy reaction is assumed to form two O ₂ + alkoxy radicals. The MEK + HO ₂ . represents the products and radicals formed from the alkoxy radical from this species. The other half is assumed to involve disproportionation, forming O ₂ + and an alcohol and carbonyl compound. These are represented by MEK and PROD ₂ .
58	This reaction is assumed to form the corresponding alkoxy radical, which is assumed to react products represented by MEK + HO ₂ .
58a	The carbonyl product formed from RO ₂ -N. is represented by PROD ₂ .
59	This operator represents the effects of peroxy radicals which react with NO to form unreactive organic nitrates (represented by XN), and also the effects of peroxy radical reactions on other species. It has no carbons.
60	This operator represents the effects of peroxy radicals which react with NO to form aromatic nitrates or nitrophenols (represented by NPHE), and also the effects of peroxy radical reactions on other species. It has six carbons.
61	The organic products from the HO ₂ reaction are represented by phenol.
62	Half this reaction is assumed to form the corresponding alkoxy radical, which is represented by phenoxy. The other half is assumed to form stable products, which are represented by phenol.
63	This reaction is assumed to form the corresponding alkoxy radical, which is represented by phenoxy.
64	Assumed to have the same rate constant and mechanism as used for the general higher acyl peroxy radical or higher PAN analogue
65	The products of the reactions of this radical and PAN analogue are based on R=ethyl. Mechanism assumed to be similar to corresponding reaction of acetyl peroxy radicals.
66	Rate parameters based on data for PPN. The activation energy is recommended by Atkinson (1994) for thermal decomposition of higher PAN analogues. The A factor is adjusted to yield the average k(298) for PPN as measured by Schurath and Wipprecht (1980) and Mineshos and Glavas (1991). The A factor recommended by Atkinson (1994) not used because it gives k(298) outside the range of both those measurements.
67	Rate constant based on k(NO ₂)/k(NO) ratio measured by Kirchner et al (1992) and the k(NO) used for general higher acyl peroxy radical species.
68	Rate constant expression based on the data of Kirchner et al (1992).
69	These are used to represent the acyl peroxy radical and PAN analogue formed from any acrolein compound, but its reactions are based on those formed from methacrolein.

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No.	Note
70	Rate parameters from Roberts and Bertman (1992), as used by Carter and Atkinson (1996).
71	The rate expression recommended by Atkinson (1997) for general alkoxy + NO ₂ reactions is $2.3 \times 10^{-11} \exp(+150/T)$. This is reduced by a factor of 1.58 to be consistent with environmental chamber data, as discussed in a separate note.
72	The effects of isobutane and t-butyl alcohol on ozone formation and radical levels in environmental chamber experiments are not consistent with predictions of models which assume the recommended rate constant ratios for the decomposition of t-butoxy radicals relative to reaction with NO ₂ . The data are better fit if the ratio is increased by a factor of 2.5. The error is assumed to be equally distributed in each rate constant, so they are both adjusted by the a factor of 1.58, which is the square root of 2.5.
73	Atkinson (1997b) recommends the high-pressure rate expression of $6.0 \times 10^{-14} \exp(-16.2/RT)$. Batt and Robinson (1987) calculate that at one atmosphere the rate constant is 79% the high pressure limit, giving an estimated rate expression of $4.74 \times 10^{-14} \exp(-16.2/RT)$. This is increased by a factor of 1.58 to be consistent with environmental chamber data, as discussed in a separate note.
74	The rate constant is based on the general recommendation of Atkinson (1994) for alkoxy + NO ₂ reactions at the high pressure limit. Nitrophenol formation has generally been assumed in this reaction (e.g., see Atkinson, 1990; Carter, 1990), presumably via some rearrangement of an initially-formed unstable adduct. However, based on lower than expected yields of nitrophenols in NO ₃ + cresol and OH + benzaldehyde systems (Atkinson, 1994), this may be an oversimplification.
75	Assumed to have the same rate constant as the reaction of HO ₂ with peroxy radicals. This may underestimate the actual rate constant.
76	This is included to avoid problems if these radicals are ever formed under conditions where both HO ₂ and NO ₂ are very low (which is considered to be unlikely under most ambient conditions), and can be considered to represent its reaction with organics present. The rate constant is arbitrary, and is such that this process becomes significant only if [NO ₂] < $\sim 3 \times 10^{-6}$ ppm and [HO ₂] < 1×10^{-5} ppm.
77	The rate constant is based on the general recommendation of Atkinson (1994) for alkoxy + NO ₂ reactions at the high pressure limit. The products of this reaction (presumed to be aromatic dinitro compounds) are expected to have very low vapor pressures and are represented as unreactive nitrogen and carbon.
78	Absorption cross sections and quantum yields recommended by IUPAC (Atkinson et al, 1997a) used. Absorption cross sections used are those given for T = 285K.
79	Rate constant assumed to be the same as used for methylperoxy + NO.
80	T=298K Rate constant recommended by IUPAC (Atkinson et al, 1979a). Temperature dependence is as estimated by IUPAC (Atkinson et al, 1979a).
81	The mechanism and rate constants are as recommended by IUPAC (Atkinson et al, 1997a, 1999). The branching ratio is for T=298K only. The overall reaction assumes the major fate of the alpha hydroxy radical is reaction with O ₂ to form HO ₂ and HCHO.
82	Rate constant and branching ratio for initial OH reaction based on IUPAC (Atkinson et al, 1997a, 1999) recommendation. The .CH ₂ OOH radical is assumed to rapidly decompose to HCHO + OH, based on its high estimated exothermicity.
83	Absorption cross sections from IUPAC (Atkinson et al, 1997a, 1999), which also recommends assuming unit total quantum yield, but gives no recommendation as to the exact mechanism. Breaking the O-O bond assumed to be the major pathway.
84	Absorption cross sections and quantum yields recommended by IUPAC (Atkinson et al, 1997a, 1999) used. Reaction assumed to occur primarily by breaking the C-CHO bond. Pathway forming molecular products from acetaldehyde is calculated to be negligible under atmospheric conditions, and is not included in the model.

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No.	Note
85	Reaction in the presence of NO _x is assumed to involve formation of CH ₃ C(O)CH ₂ O., after one NO to NO ₂ conversion. Based on the data of Jenkin et al (1993), this radical is believed to rapidly decompose to HCHO + CH ₃ CO.
86	Absorption cross sections and quantum yields used are those recommended by IUPAC (Atkinson et al, 1997a) except as noted. The reported quantum yields at 230 and 330 are expected to be high and an estimated correction was made as discussed by Carter et al (1993b). The corrected quantum yield data for wavelengths less than 290 nm were then fit to a smooth curve to estimate the quantum yields for higher wavelengths, with no weight being given to the highly uncertain 330 nm point. As discussed by Carter et al (1993b), using these corrections results in better fits of model calculations to environmental chamber experiments involving acetone.
87	Absorption cross sections from Plum et al (1983), as recommended by IUPAC (Atkinson et al, 1997a, 1999) in the case of glyoxal.
88	For the low wavelength band, a constant quantum yield of 0.4 is assumed, based on data of Langford and Moore (1984). For the high wavelength band, quantum yield is assumed to decrease linearly to zero at the threshold wavelength of 418 nm, starting at a "falloff" wavelength, which is adjusted to yield fits to chamber data for acetylene - NO _x and acetylene reactivity experiments, as discussed by Carter et al (1997c). "Best fit" falloff wavelength of 380 nm used. Note that this gives overall quantum yields which are ~1.4 times higher than overall quantum yield reported by Plum et al (1983) for conditions of those experiments. Although use of acetylene reactivity data is a highly indirect way to obtain glyoxal quantum yields, it is considered to be a less uncertain way to estimate radical quantum yields than the data of Plum et al (1993), which uses a UV-poor light source and only measures rates of glyoxal decay.
89	Plum et al (1983) observed 13% formaldehyde yield in photodecomposition, so overall quantum yield adjusted to give this yield relative to the radical forming process for the spectral distribution of those experiments. A wavelength-independent quantum yield is used because of lack of information on wavelength dependence.
90	Product distribution based on the data of Niki et al (1985), as discussed by IUPAC (Atkinson et al, 1987a). Product distribution is calculated for 1 atm air at 298K.
91	Assumed to have the same rate constant and mechanism as the analogous reaction with acetaldehyde.
92	Absorption cross sections obtained from Moortgat (personal communication, 1996). These are essentially the same as those recommended by IUPAC (Atkinson et al, 1997a, 1999), except slightly better resolution. Photolysis at the low wavelength band is assumed to have unit quantum yields, based on data for biacetyl. Photolysis above the cutoff wavelength of 421 nm (Atkinson et al, 1977a) is assumed to have zero quantum yields. For the rest of the high wavelength region, the wavelength dependence was derived by assuming the quantum yields decline linearly from 1 at 344 nm to 0 at a wavelength (407 nm) which was adjusted to be such that the calculated overall quantum yields for the conditions of the experiments of Plum et al (1983) agreed with the overall quantum yield they observed experimentally. The quantum yields recommended by IUPAC (Atkinson et al, 1999) lack sufficient wavelength resolution to be useful for modeling.
93	Assumed to have unit quantum yield at low wavelength band based on data cited by Atkinson (1994). For the high wavelength band, the quantum yields were assumed to decline linearly from 1 at 350 nm to 0 at a wavelength (420 nm) which was adjusted to be such that the calculated overall quantum yields for the conditions of the experiments of Plum et al (1983) agreed with the overall quantum yield they observed experimentally.
94	Rate constant recommended by Atkinson (1989).

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No.	Note
95	Abstraction from HCO estimated to occur 75% of the time, which is intermediate between that estimated from the rate constant derived for the analogous reaction of methacrolein and the rate constant estimated using the structure-reactivity method of Atkinson (1987). OH addition to the terminal vs internal position is assumed to occur with a 2:1 ratio, based on data for the reaction of OH with propene.
96	Except as indicated by other footnotes, the overall reaction mechanism was derived using the general estimation methods for atmospheric reactions of alkyl, alkyl peroxy, and alkoxy radicals and the automated mechanism generation system as discussed by Carter (1999).
97	$\text{CH}_2=\text{CHC}(\text{O})\text{OO}\cdot$. Is represented by MA-RCO3.
98	The T=298K rate constant is that recommended by Atkinson (1994). The activation energy is estimated to be the same as that for the reaction of O3 with methacrolein.
99	The initially formed ozonide is assumed to decompose to glyoxal + excited HCHO_2 and to formaldehyde + excited $\text{HC}(\text{O})\text{CHO}_2$ with equal probability.
100	The excited HCHO_2 biradical is assumed to react as recommended by Atkinson (1997) based on data for the O3 + ethene system, i.e., 37% stabilization, 12% decomposition to $\text{HCO} + \text{OH}$, 13% decomposition to $\text{CO}_2 + \text{H}_2$, and 38% decomposition to $\text{CO} + \text{H}_2\text{O}$. Note that this is different than used for this species when formed in the isoprene products mechanisms of Carter and Atkinson (1996) and Carter (1996).
101	The reactions of the excited $\text{HC}(\text{O})\text{CHO}_2$ biradical are estimated by analogy to the mechanism assumed for the reactions of excited CH_3CHO_2 biradicals, as discussed elsewhere (see Carter, 1999B). This is as follows: 34% stabilization, 52% decomposition to $\text{HCO} + \text{CO} + \text{OH}$, and 14% decomposition to $\text{HCHO} + \text{CO}_2$.
102	Ratios of T=298K rate constants for acrolein relative to ethylene assumed to be the same as that for methacrolein relative to propylene. Assumed to have same A factor as NO_3 + propene reaction.
103	NO_3 radical addition assumed to occur primarily at the least substituted position.
104	The $\text{HCOCH}(\text{O})\cdot\text{CH}_2\text{ONO}_2$ radical is expected to decompose primarily to $\text{HCO}\cdot + \text{HC}(\text{O})\text{CH}_2\text{ONO}_2$. The latter is represented by $\text{RCHO} +$ "lost nitrogen".
105	Rate constant estimated from linear correlation between log k for OH and O3P reaction. Chamber data for C_{3+} alkenes are better fit by models assuming O3P reactions with C_{3+} species do not form radicals. Stable products represented by the lumped higher aldehyde or ketone, depending on type of product(s) expected to be formed.
106	Acrolein absorption cross sections from Gardner et al. (1987).
107	Overall quantum yield for decomposition to radicals, assumed to be independent of wavelength, was adjusted to optimize fits of model simulations to acrolein - NOx chamber experiments carried out by Carter et al (1987). The photodecomposition mechanism is assumed to be analogous to that derived by Carter and Atkinson (1996) for methacrolein, with fragmentation to $\text{HCO}\cdot + \text{CH}_2=\text{CH}\cdot$, $\text{CH}_2=\text{CHC}(\text{O})\cdot + \text{H}\cdot$, and $\text{CH}_3\text{-CH}(\text{carbene}) + \text{CO}$ occurring with approximately equal probability.
108	The carbene is assumed to react with O2 to form the excited CH_3CHO_2 biradical, which is assumed to react in the same way as assumed in the ozone + propene mechanism (Carter, 1999b). NROG represents the methane formed in this reaction.
109	The vinyl radicals are assumed to react with O2 to form $\text{HCO}\cdot + \text{HCHO}$ based on the data of Slagle et al (1984).
110	The rate constant and mechanism of Carter and Atkinson (1996) was used with no significant changes (except as indicated in other footnotes, if applicable). Some minor changes in product yields may result in some cases from use of the general mechanism estimation system (Carter, 1999a) to generate the overall reaction scheme.
111	MEK is used to represent hydroxyacetone.

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No.	Note
112	The vibrationally excited $\text{HCOC}(\text{CH}_3)\text{CO}_2$ biradicals are assumed to rearrange and decompose to $\text{HCOC}(\text{O})\text{CH}_2 + \text{OH}$, where the former forms $\text{HCOC}(\text{O}) + \text{HCHO}$ after O_2 addition and NO to NO_2 conversion. RCO-O_2 is used to represent $\text{HCOC}(\text{O})\text{OO}$ in this reaction. Vibrationally excited $\text{CH}_3\text{C}(\text{O})\text{CHO}_2$ is assumed to rapidly convert to $\text{HCOC}(\text{CH}_3)\text{CO}_2$ as discussed by Carter and Atkinson (1996).
113	The product $\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{ONO}_2$ is expected to be relatively unreactive and is represented as "lost nitrogen" + 3 "lost carbons".
114	The overall quantum yield was reoptimized to fit the same data as discussed by Carter and Atkinson (1996). In the case of methacrolein, the changes to the other portion of the mechanism resulted in an ~14% increase in the best fit overall quantum yield compared to that derived by Carter and Atkinson (1996). In the case of MVK, the best fit overall quantum yield decreased by a factor of 5.
115	(number skipped)
116	Rate constant recommended by Atkinson (1994).
117	The parameterized mechanism is estimated by analogy to the parameterized mechanism derived for cresols (see footnotes for $\text{OH} + \text{cresol}$ reaction).
118	In absence of definitive data concerning this reaction, the same mechanism is used as assumed by Carter (1990). However, see footnotes concerning phenoxy reactions.
120	The mechanism for ROOH is based on reactions estimated for n-propyl hydroperoxide.
121	Reaction at the OOH position is assumed to be as fast as in CH_3OOH . Reaction at the 1-position is estimated to be $\sim 7 \times 10^{-12}$ (i.e., $\sim 2/3$ of the time) based on comparing rates of analogous reactions for methanol, ethanol, and CH_3OOH (IUPAC, 1997a, 1999). The alpha-hydroperoxy radicals are assumed to decompose rapidly to OH and the carbonyl on the basis of estimated high exothermicity. Reaction at the 2- or 3-positions are estimated to occur no more than ~10% of the time and are neglected.
122	Reaction assumed to occur with the same rate and analogous mechanism as methyl hydroperoxide.
123	The mechanism for RCHO is based on reactions estimated for propionaldehyde.
124	OH reactions at various positions in the molecule estimated using the group-additivity methods of Kwok and Atkinson (1995), as updated by Kwok et al (1996).
125	Assumed to have same rate constant and analogous mechanism as reaction of acetaldehyde.
126	The absorption coefficients used for MEK are from Moortgat (Private communication, 1996). The overall MEK quantum yield of 0.1 was derived from fits to UNC chamber data as determined by Carter et al (1986), and is consistent with results of MEK reactivity experiments carried out in our laboratories (Carter et al, 1999a). The reaction is assumed to proceed primarily by breaking the weakest CO-C bond.
127	Mechanism for RNO_3 based on that estimated for 2-pentyl nitrate.
128	Total OH rate constant estimated using group additivity method of Kwok and Atkinson (1995).
129	MEK represents 2-pentanone, RCHO represents propionaldehyde, 2-nitro propionaldehyde and various C5 nitro-aldehydes, RNO_3 represents various C5 nitro ketones, and PROD2 represents 5-hydroxy-2-pentanone.
130	Absorption cross sections given by IUPAC (Atkinson et al, 1997a, 1999) for isopropyl nitrate are used. As discussed by IUPAC (Atkinson et al, 1999), the quantum yield is expected to be near unity for formation of NO_2 . Other products based on subsequent reactions estimated for 2-pentoxy radicals. PROD2 represents 5-hydroxy pentanone, MEK represents 2-pentanone, and RCHO represents propionaldehyde.
131	Mechanism for PROD2 based on that for 5-hydroxy-2-pentanone.
132	RCHO represents 3-oxo butyraldehyde, 2-oxo propionaldehyde and 3-hydroxy propionaldehyde. RCO-O_2 represents $\text{HOCH}_2\text{CH}_2\text{C}(\text{O})\text{OO}$.

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No.	Note
133	Assumed to photolyze with the same rate absorption cross section and quantum yields as used for MEK. Reaction assumed to involve initial formation of $\text{CH}_3\text{C}(\text{O})\cdot + \text{HOCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\cdot$, with the latter reacting as estimated using the general procedures (Carter, 1999). RCHO represents primarily 3-hydroxy propionaldehyde.
134	The parameterized mechanism is based on that used by Carter (1990), but was reoptimized to fit the NO, ozone, PAN, and cresol data in the o-cresol - NO _x experiment EC281.
135	Absorption coefficients are from Majer et al (1969). The overall quantum yield derived by Carter (1990), which are based on model simulations of benzaldehyde decay rates in SAPRC evacuable chamber experiments, is used. Because of lack of data, the quantum yield is assumed to be independent of wavelength. The products formed from benzaldehyde photolysis are unknown, except that both radical formation and benzene formation appear to be minor (Carter, 1990). This benzaldehyde photolysis mechanism gives reasonably good model simulations of benzaldehyde - NO _x experiments recently carried out in the CE-CERT xenon Teflon chamber (Carter et al, 1998a).
136	T=298K rate constant recommended by Atkinson (1994). Temperature dependence estimated by assuming the reaction has the same A factor as the reaction of NO ₃ with acetaldehyde.
137	Assumed to have the same rate constant as the reaction of NO ₃ with phenol. Reaction with NO ₃ is assumed to dominate over reaction with OH radicals and other loss processes.
138	DCB1 is a lumped species used to represent the unsaturated carbonyl products formed in the ring opening reactions of benzene and naphthalene. Its mechanism is largely parameterized, but is based roughly on estimated reactions of 2-butene-1,3-dial.
139	The rate constant is based on data of Bierbach et al (1994). The reaction is assumed to proceed via addition of OH to double bond, followed by decomposition of the alkoxy radical to HCO and $\text{HC}(\text{O})\text{CH}(\text{OH})\text{CHO}$, where the latter is represented by RCHO .
140	The photolysis action spectra of these products are assumed to be similar to that for acrolein, so the absorption cross sections of acrolein are used, with a wavelength-independent overall quantum yield. The overall quantum yield is adjusted to optimize fits of model simulations to the benzene - NO _x experiments used in the optimization of the previous version of the mechanism by Carter et al (1997a). The photolysis is represented as initially forming $\text{HCO}\cdot + \cdot\text{CH}=\text{CHCHO}$, where the latter forms $\text{HCOCH}(\cdot)\text{CHO}$ after O ₂ addition and NO to NO ₂ conversion, then $\text{HCO} + \text{glyoxal}$ after one more O ₂ addition and NO to NO ₂ conversion.
141	The rate constant is based on the data of Bierbach et al (1994). The reaction is assumed to involve initial formation of glyoxal and $\text{HC}(\text{O})\text{CHO}_2$.
142	DCB2 and DCB3 represent the highly photoreactive unsaturated dicarbonyl product formed from the ring-opening reactions of the alkylbenzenes. To fit chamber data using differing light sources, they are represented by two species, which differ only in their action spectra and overall quantum yields, with the action spectrum of DCB2 being like methyl glyoxal, and that of DCB3 being like acrolein, and with the overall quantum yields adjusted separately to fit chamber data. Its reactions are based roughly on estimated reactions of a 5-carbon compound with general structure $\text{XC}(\text{O})\text{CX}=\text{CXC}(\text{O})\text{X}$, where X can be H or alkyl.
143	Assumed to have the same rate constant as used for DCB1. Mechanism represented as OH adding to double bond in $\text{XC}(\text{O})\text{CX}=\text{CXC}(\text{O})\text{X}$, with alkoxy radical decomposing to $\text{CH}_3\text{CO}\cdot$ and $\text{XCO}-\text{CH}(\text{OH})-\text{CXO}$, the latter being represented by RCHO . Note that the general alkoxy radical estimation method (Carter, 1999) predicts that alkoxy radicals like $\text{RCH}(\text{OH})\text{CH}(\text{O}\cdot)\text{C}(\text{O})\text{R}'$ will decompose primarily to $\text{RCH}(\text{OH})\text{CHO} + \text{RC}(\text{O})\cdot$.

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No.	Note
144	The overall quantum yields for DCB2 and DCB3 were optimized to give best fits of model simulations of NO oxidation, O ₃ formation and xylene consumption in m-xylene - NO _x chamber runs with various light sources, and also to mini-surrogate - NO _x runs. The DCB2 and DCB3 quantum yields had to be adjusted as well as the yields of these products from m-xylene to best fit the data for the various light sources, and also to fit the results of the mini-surrogate as well as the m-xylene only runs. (For the other aromatics, only the DCB2 and DCB3 yields are optimized.) The mechanism is represented as the photolysis of XC(O)CX=CXC(O)X forming XCO. + .CX=CXC(O)X, which forms XCOC(.)XC(O)X after an NO to NO ₂ conversion, then forms XC(O)C(O)X + XCO. after another. Half of the XCO. is CH ₃ CO., the other half is HCO. Half the dicarbonyl is glyoxal, the other half is methyl glyoxal.
145	DCB4 is used to represent ring opening products formed from the reactions of OH radicals with alkylbenzene which are not photoreactive, such as believed to be the case for unsaturated diketones (Bierbach et al, 1994). Their reactions are represented based roughly on the estimated mechanism for 3-hexene 2-5-dione.
146	Assumed to have a similar rate constant as used for DCB1. Although the mechanism estimated based on the structure of 3-hexene 2-5-dione would be similar to those used for DCB2 and DCB3, somewhat better fits to p-xylene and 1,2,4-trimethylbenzene chamber data are obtained if this reaction is assumed to form products analogous to those estimated for DCB1.
147	Rate constant estimated based on data of Bierbach et al (1994). Mechanism estimated based on O ₃ + 3-hexene 2,5-dione forming methyl glyoxal + CH ₃ C(O)CHO ₂ .
148	As discussed by Carter (1996), isoprod is the "four product" lumped isoprene product species whose mechanism is derived by lumping rate constant and product parameters for a mixture of 30% hydroxymethacrolein, and 70% equal amounts of cis and trans HCOC(CH ₃)=CHCH ₂ OH and HCOCH=C(CH ₃)CH ₂ OH. These proportions are based on the estimated yields of these products in the reactions of OH with isoprene (Carter and Atkinson, 1996), which are represented by ISOPROD in the four product condensed mechanism (Carter, 1996). The other footnotes refer to the estimated mechanisms for these four individual compounds which were used to derive the lumped ISOPROD mechanism. RCHO, PROD2, MA-RCO3, etc. are used to represent various compounds as indicated in the descriptions of these lumped model species. See Carter and Atkinson (1996) for the specific compounds which can be formed in the various reactions of these species.
149	The excited CH ₃ C(O ₂)CH ₂ OH biradical is assumed to react primarily via rearrangement to the unsaturated hydroperoxide followed by decomposition to OH radicals and the corresponding carbonyl compound, as is assumed in the general alkene mechanism (Carter, 1999b). Two possible such rearrangements can occur in the case of this biradical, one to CH ₂ =C(OOH)CH ₂ OH, which decomposes to OH + HOCH ₂ C(O)CH ₂ ., and the other to HOCH=C(OOH)CH ₃ , which decomposes to OH + CH ₃ C(O)CH(.)OH. The relative importances of the competing rearrangements in such cases is estimated by assuming they are approximately proportional to the estimated OH abstracting rate constant from the H-donating group (Carter, 1999b). Based on this, the overall reaction is estimated to be OH + 0.04 HOCH ₂ C(O)CH ₂ . + 0.96 CH ₃ C(O)CH(.)OH, with the subsequent reactions of these radicals being derived by the general estimation methods (Carter, 1999a).
150	All the species represented by ISOPROD are assumed to have the same overall photolysis rate as used for methacrolein.

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No.	Note
151	Isoprene mechanism used is based on the "four product" condensed isoprene mechanism of Carter (1996) which in turn is based on the detailed isoprene mechanism of Carter and Atkinson (1996). The rate constants and the major initial reaction pathways are the same as used in those mechanisms. Some minor changes in product yields resulted in some cases from use of the general mechanism estimation system (Carter, 1999a) to generate the overall reaction schemes, or as indicated in other footnotes.
152	The overall nitrate yield is slightly higher than the adjusted nitrate yields in the Carter and Atkinson (1996) mechanism because the mechanism generation system included some nitrate formation from peroxy radicals formed in secondary reactions. Although the yields were not readjusted, the mechanism still gives satisfactory fits to the isoprene chamber data used in the nitrate yield adjustments by Carter and Atkinson (1996).
153	The excited $\text{CH}_2=\text{CHC}(\text{O}_2)\text{CH}_3$ and $\text{CH}_2=\text{C}(\text{CH}_3)\text{CHO}_2$ biradical reactions are the same as given by Carter and Atkinson (1996), except that the $\text{CH}_2=\text{CHC}(\text{O})\text{O}_2$ formed from the former is represented by MA-RCO3, and the propene formed from the latter is represented by PROD2.
154	All the organic products formed in this reaction are represented by ISOPROD. A small amount of nitrate formation is estimated to occur from the reactions of the substituted peroxy radicals with NO (Carter, 1999a).
155	PROD2 is used to represent the various isoprene oxide products. And MA-RCO3 is used to represent $\text{CH}_2=\text{CHC}(\text{O})\text{OO}$. Note that this mechanism, which is based on that of Carter and Atkinson (1996) is inconsistent with the mechanisms for the reactions of O^3P with the other higher alkenes, which are assumed not to form radical products. However, assuming no radical formation in the reaction of O^3P with isoprene results in somewhat degraded model performance in simulations of the results of the isoprene experiments discussed by Carter and Atkinson (1996).

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